Nanoscale Disorder in Crystalline Materials

Scientific Achievement

We are developing instrumentation and analysis tools to maximize the potential of single crystal diffuse scattering as a powerful probe of complex disorder. In order to obtain efficient measurements over large volumes of momentum space while eliminating inelastic scattering, we have designed a neutron scattering white-beam diffractometer that utilizes cross correlation to provide energy discrimination. A prototype is currently being installed at the Intense Pulsed Neutron Source and will be used to test the advantages of this novel concept over the conventional methods. We have also started whole experiment simulations, including both instrument components and the sample itself, to support the tests and ultimately the design of a dedicated single crystal diffractometer to be built at the Spallation Neutron Source. We have already solicited advice from international experts, established an Instrument Advisory team, and submitted a Letter of Intent to submit a proposal to the Experimental Advisory Committee of the Spallation Neutron Source.

In parallel with this work, we have also tested and improved the rotation method using area detectors to measure single crystal diffuse X-ray scattering over large volumes of reciprocal space. We found that the limitations of this technique encountered using lower energy X-rays are overcome by using energies above 60keV. Such high energy X-rays are particularly crucial for avoiding complicated corrections due to sample absorption, air scattering, and fluorescence background as well as for obtaining sufficiently large momentum coverage with a single detector setting.

Significance

Many emerging phenomena with technological potential are governed by complex disorder and nanoscale self-organization, such as stripes, phase separation and dimerization. The most powerful probe of such disorder in crystalline materials on the 1-10nm length scale is neutron and x-ray diffuse scattering. This technique has, however, so far been limited to the study of a few specific problems of limited complexity because of the technical difficulties both in obtaining reliable data with existing instrumentation and in subsequent modeling of such data with existing analysis tools. The development of the rotation method using high energy synchrotron X-rays already allows us to obtain very efficiently high quality data over the large volumes of reciprocal space required for accurate modeling of the local structure. Our development of novel concepts for efficient energy discrimination at pulsed neutron sources will enable the separation of inelastic processes such as thermal diffuse scattering and open the path for single crystal diffuse scattering to become a key technique for studying emerging complex phenomena. A review of the prospects and challenges of single crystal diffuse scattering can be found in S. Rosenkranz and R. Osborn, Neutron News 15, 21 (2004).

Performers

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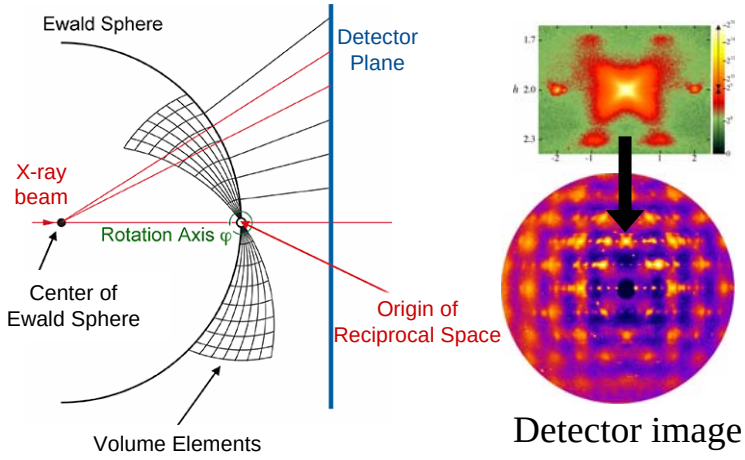
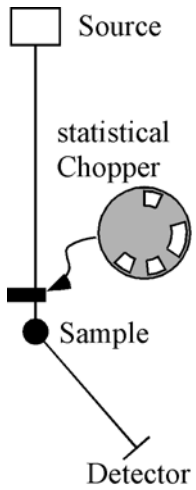
Nanoscale Disorder in Crystalline Materials

- Develop single crystal diffuse scattering to probe local distortions and short range correlations
- Use it in ongoing research program to study emerging complex phenomena



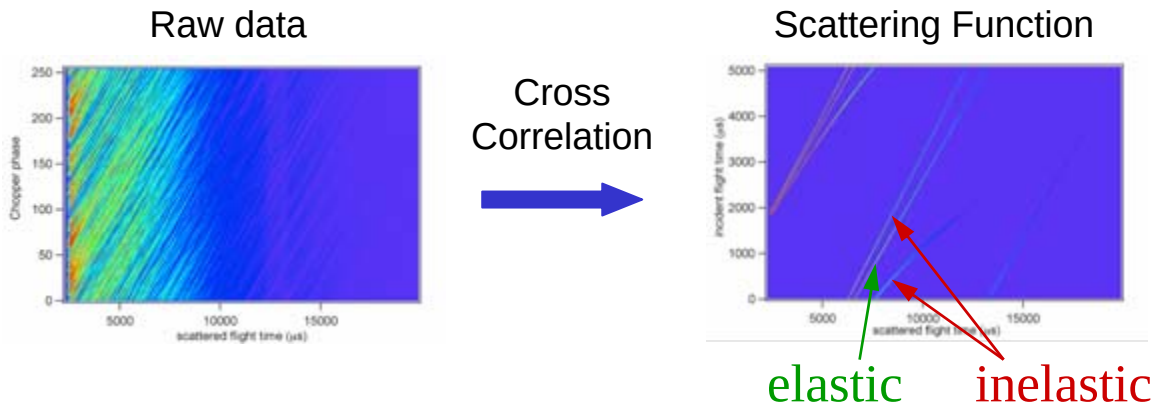
Synchrotron X-rays

- Rotation method using high energy synchrotron X-rays and area detectors provides very efficient coverage of large volumes of diffuse scattering



Neutrons

- A correlation chopper provides both energy discrimination and efficient coverage of momentum space



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